

Pyrrolidine
123-75-1 | DTXSID3059559

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.72 days

Global applicability domain: Inside

Local applicability domain index: 6.21e-01

Confidence level: 9.20e-01

Nearest Neighbors from the Training Set

Image not found

Methylcyclopentane

Measured: 24.3

Predicted: 4.41

Image not found

1,3-Dimethylcyclopentane

Measured: 24.3

Predicted: 4.08

Image not found

1,2-Dimethylcyclopentane

Measured: 24.3

Predicted: 4.46

Image not found

Hexane, 2,2,5-trimethyl-

Measured: 777

Predicted: 17.4